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Theoretical Computations of Transition Metal NMR Chemical Shifts

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Density functional theory (DFT) is now well etablished for the computation of NMR properties including chemical shifts of transition-metal compounds [1]. In most cases the B3LYP combination of density functionals is better suited than others to describe the shifts of the metal nuclei, $\delta(^{95}\mathrm{Mo})$ being the only exception so far [1]. We have now extended the series of examined nuclei to include ^{49}Ti [2] and ^{99}Ru chemical shifts [3], both of which are well reproduced with B3LYP (Figure 1) .

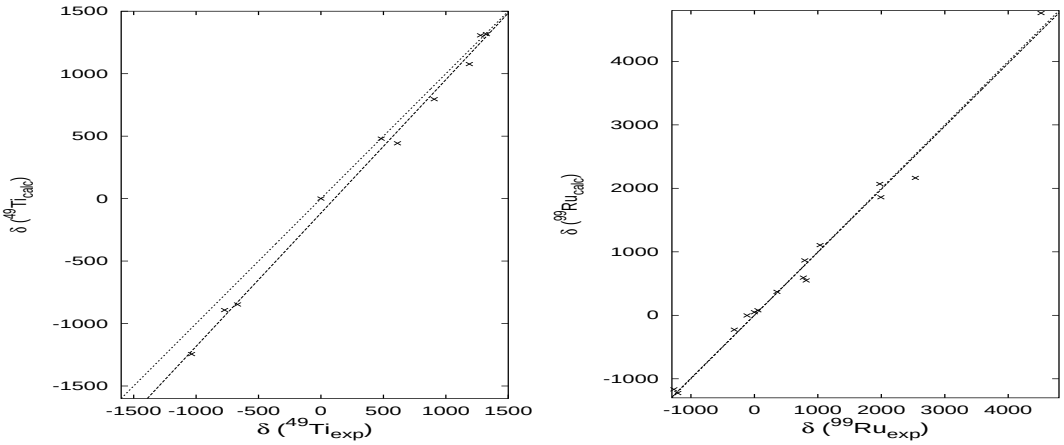

Figure 1: Computed (GIAO-B3LYP) versus experimental transition-metal chemical shifts; left: ^{49}Ti, right: ^{99}Ru. (dotted: ideal slope = 1, dashed: linear fit)

References

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